

Opportunities and Leverage

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Questions for Thursday Breakout

1. Based on the workshop proceedings to date, where do you see opportunities for new innovations to impact multiphysics simulations, especially in:
 - a. Algorithms
 - b. Software engineering
 - c. Hardware
2. What challenges do you see that have not been well handled by current *theory*, methods, or software?
3. Are there innovations that have been very successful in one application that can be applied to others?
4. What multiphysics integration would your community like to perform today that by conventional wisdom is out of reach, but might be crackable with a specific breakthrough?

Are there innovations successful in one application
that can be applied to others?
[multiphysics]

- Design paradigm from Bell's BOXLIB: abstraction of refinement from local nested h -type mesh refinement to generalized local refinement, including model refinement
 - needs machinery analogous to timestep control and refluxing
- Separation of concerns: physics from solver
 - If the solver is intermingled with the physics, it is difficult for the mathematician to find it and difficult to try innovations in solvers
 - A low-level but common and successful interface between the physics and the solver is a subroutine like PETSc's "FormFunction" that evaluates a local piece of the vector-valued residual or rate $F(u)$

Are there innovations successful in one application
that can be applied to others?
[multiphysics]

- Error/iteration control of the Gauss-Seidel loop in time-evolving systems: measure cross-variable sensitivities to estimate degree of coupling
- Coding for extreme computers: learn software techniques from solver groups
 - Solver libraries implement global distributed data structures in ways that respect communication (neighbor tracking, aggregation, hiding) and memory layouts (cache and register blocking, coloring)
 - Applications may want to control their own data structures but can learn much from a performance-oriented general algebraic framework to enable this. In multiphysics, if all apps control separate data structures, there may be little chance for performance at extreme scale

Are there innovations successful in one application
that can be applied to others?
[monophysics]

- Tricks from audience members not otherwise discussed:
 - Evaluation of $F(u)$ and $F'(u)v$ simultaneously from Real and Imaginary parts of a complex-valued residual evaluation
 - Capturing of stationary periodic behavior in $u(t+T) \leftarrow P(u(t), T)$ by applying Newton to the fixed point $F(u) = u - P(u, T)$
 - Nonlinear acceleration techniques that solve directly for the correction δu , rather than for u
- Physics-based preconditioning (examples: Knoll & Chacon – MHD, climate)
- Jacobian-free acceleration (example: Wigton et al – TRANAIR)

What challenges have not been handled by current theory, methods, or software?

- Connection between discrete and continuum domains
 - How are errors controlled at this interface? How to understand whether information loss in going from fine to coarse grain is acceptable?
- Interpolation between continua represented on nonconforming meshes (interfaces and bulk)
 - OVERLINK is said to do this well
 - May need system that knows underlying geometry of interface, not just the discrete meshes
- Time-step selection that guarantees desired accuracy
- Time-step selection that guarantees stability of the multiphysics combination of two physics components whose CFL stabilities are well characterized
 - Linearized stability approachable through analysis of off-diagonal blocks

What challenges have not been handled by current theory, methods, or software?

- Time-splitting that offers greater than second-order accuracy
 - Theory requires operators to commute, which may be the case in ADI, but is not the case in practical multiphysics
 - Richardson Extrapolation can be used to obtain higher order, but it is difficult to control if one operator is stiff
- Backtracking control in Newton methods
 - Ordinarily, backtracking is designed to prevent stepwise increase in residual; however strategy fails when nonlinear function increases in norm to get from one local minimum to another – different globalization criteria needed for cases where current approaches fail.

What multiphysics seems out of reach but crackable with specific breakthroughs?

- ‘If we build it they will come’
 - Often apps people are attracted to something that can be demonstrated; OTOH intuition and heurism from apps often lead theory
 - Apps people often learn their numerics in home departments
- Need for compact examples for practitioners and students that can be appreciated without too much exposure to particular physics
- To optimize science done by computation (per \$, Watt, person) we need several factors coming from num. analysis
 - Convergence rates as a function of discretization parameters
 - Complexity estimates in terms of convergence rates and cost per iteration
 - Resource requirements that accompany flops
 - If we can't define the objective function with some rigor, we cannot optimize it

Where would innovations in SW engineering impact multiphysics simulations?

- Hardware has made flops relatively cheap – what new thinking does this offer multiphysics?
 - Time-parallel methods probably not, since they presume extra memory
 - Predictor-corrector algorithms may be good, since prediction costs flops but uses little memory (explicit)
 - Aitken-type Extrapolation to predict messages to be received in the future relative to opportunity to do some flops
- Small/fast checkpointing based on user-specified minimum state
- Stochastic error analysis perhaps newly affordable
- Less synchronous algorithms useful
 - Need to beat back to causal limits to asynchronous communications
 - Today we synchronize artifactually and too much from loop structures
 - However, asynchronous algorithms typically compromise robustness
- Parallel meshing/remeshing algorithms are as important or more as in monophysics
- Trans-dimensional interpolation is a new consideration